Convection 2D

August 22, 2007

1 Equations

1.1 Mass conservation

$$\frac{\partial c_i}{\partial t} = -\vec{\nabla}.\vec{N}_i + R_i \tag{1}$$

with

$$\vec{N}_i = c_i \vec{v} - \sum_j D_{ij} \vec{\nabla} c_j - w_i c_i \vec{\nabla} U \tag{2}$$

1.2 Poisson's equation

$$\vec{\nabla}^2 U + \frac{F}{\epsilon} \sum_i z_i c_i = 0 \tag{3}$$

1.3 Butler-Volmer kinetics

$$v = k_{ox} \exp\left[\frac{\alpha_{ox} n F}{RT}(V - U)\right] c_{red} - k_{red} \exp\left[-\frac{\alpha_{red} n F}{RT}(V - U)\right] c_{ox} \tag{4}$$

2 Element matrix

2.1 Convection

2.1.1 Fluctuation in node

$$\Delta c_i^m = \sum_e \alpha_e^m \Phi_e$$

2.1.2 Element contribution to fluctuation in node

$$\begin{aligned} \Phi &= \textstyle\int_S -\vec{v}.\vec{\nabla} c_i dS \\ &= -\left(\frac{\vec{n}^1 c_i^1 + \vec{n}^2 c_i^2 + \vec{n}^3 c_i^3}{2}\right).\vec{v}_{av} \\ &= -\left(k^1 c_i^1 + k^2 c_i^2 + k^3 c_i^3\right) \end{aligned}$$

- One target (e.g. node 1)

$$\alpha^1 = 1$$

$$\alpha^2 = \alpha^3 = 0$$

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \end{array}\right\} = \left[\begin{array}{ccc} -k^1 & -k^2 & -k^3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \end{array}\right\} \tag{5}$$

- Two target: LDA-scheme (e.g. nodes 1 and 2)

$$\alpha^1 = -\frac{k^1}{k^3}$$

$$\alpha^2 = -\frac{k^2}{k^3}$$

$$\alpha^3 = 0$$

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \end{array}\right\} = \left[\begin{array}{ccc} \frac{\left(k^1\right)^2}{k^3} & \frac{k^1 k^2}{k^3} & k^1 \\ \frac{k^2 k^1}{k^3} & \frac{\left(k^2\right)^2}{k^3} & k^2 \\ 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \end{array}\right\} \tag{6}$$

- Two target: N-scheme (e.g. nodes 1 and 2)

Note: the distribution coefficients are undefined!

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \end{array}\right\} = \left[\begin{array}{ccc} -k^1 & 0 & k^1 \\ 0 & -k^2 & k^2 \\ 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \end{array}\right\} \tag{7}$$

2.1.3 Examples: binary electrolyte

- One target (node 1)

$$\left\{\begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \end{array}\right\} = \left[\begin{array}{ccccccccc} -k^1 & 0 & 0 & -k^2 & 0 & 0 & -k^3 & 0 & 0 \\ 0 & -k^1 & 0 & 0 & -k^2 & 0 & 0 & -k^3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \end{array}\right\} \tag{8}$$

- Two target: N-scheme (nodes 1 and 2)

$$\left\{\begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \end{array}\right\} = \begin{bmatrix} -k^1 & 0 & 0 & 0 & 0 & 0 & k^1 & 0 & 0 \\ 0 & -k^1 & 0 & 0 & 0 & 0 & 0 & k^1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -k^2 & 0 & 0 & k^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -k^2 & 0 & 0 & k^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \left\{\begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \end{array}\right\} \tag{9}$$

3 Element jacobian

3.1 Convection

Zero contribution.